Subject index

Ab initio algorithms 337
Active orbitals 81
Acyclic walks 403
ANO 419

Basis set expansion 141
Basis set limit 361
Basis set polarization approach 123
Bond border index 377
Bond distances 81

Chemical distance 65
Chemical reactions 183, 191, 199, 241
Cluster model 413
CNDO approximation 141
Complex ion 349
Complexity 379
Computer memory 155
Convergence 93
Correlated molecular wave functions 419
Coupled cluster approach 1
CPHF 115
C programming language 1
Cross sections 183, 191
Crystal field 349

Data streams 155
Density functionals 373
Dipole moments and polarizabilities of the second-row hydrides 123
Direct methods 115
Discrete polynomials 283
Dissociation channels 105
Distributed memory 191, 323

Electron affinity 419
Electron correlation 361
Electron repulsion integrals 115
Electronic spectrum 105
Electronic structure 1
Electrostatic potentials 373
Elimination tree 169
Excitation energies 105
Exotic atoms 373

FH_2 183
Finite difference boundary value method 241

Gaussian elimination 169
Geometry optimization 105
Graph theory 65

Hückel theory 403
Hydroxyl ion $A^3\Pi$ state 81
Hyperspherical coordinates 183, 225

Inelastic and reactive scattering 283
Instruction streams 155
Integral equations 297
Integral transformation 115
Ionic radii 373
Ionization potential 419

Jug's index 377

Lattice animals 379
Length representation 93
Ligand polarization 349
Localized orbitals 389

Matrix elements 43, 53
Maximum bond order 377
Memory management 241
Metal surfaces 413
Molecular dynamics 271
Molecular electric properties 123
Molecular orbitals 115
Moments 403
MP2 115
Multifrontal method 169

Outgoing wave variational principle 241
Oxygen chemisorption 413

Parallel algorithms 337
Parallel computer architectures 155
Parallel computing 175, 191, 199, 297, 323
Parallelization 169
Parallel super-computer 225
Partial cross sections 313
Phosphorus(I) oxide 105
Polarizability 419
Polarization corrected potential 141
Polarized basis sets 123
Processor granularity 155
Proton affinity 141

Quantum dynamics 175, 183, 199, 241, 271
Quantum eigenvalues 215
Quasiclassical trajectories 323

Rate constants 323
Reaction distance 65
Reaction graphs 65
Reactive Infinite Order Sudden Approximation 191
Reactive scattering 225
Reactive scattering resonance 313
Resonance behaviour 313
Resonance energy 403
Restricted active space (RAS) SCF 81

Schrödinger equation 1
Second quantization equations 1
Second row atoms 419
Shape analysis 379
Shared memory 191, 323
Shared memory computers 337
Similarity 379
Sparse linear equations 169
Spherical harmonics 283
Subduction coefficients 43
Symmetry 115

Time-dependent quantum theory 313
Transition metal molecules 389
Transition moments 93
Two-electron integrals 115

Vectorization 169
Velocity representation 93
Vibrational coordinates 349
Vibrational energies 215
Vibrational frequencies 105
Vibronic intensities 349

Wave packets 175, 297
Weyl tableau 43, 53
Wiberg index 377